1 Introduction

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Optimization problems occur very frequently in physics. Some of them are easy to handle with conventional methods also used in other areas such as economy or operations research. But as soon as a huge number of degrees of freedom are involved, as is typically the case in statistical physics, condensed matter, astrophysics and biophysics, conventional methods fail to find the optimum in a reasonable time and new methods have to be invented. This book contains a representative collection of new optimization algorithms that have been devised by physicists from various fields, sometimes based on methods developed by computer scientists and mathematicians. However, it is not a mere collection of algorithms but tries to demonstrates their scope and efficiency by describing typical situations in physics where they are useful.

The individual articles of this collections are self-contained and should be understandable for scientists routinely using numerical tools. A more basic and pedagogical introduction into optimization algorithms is our book on *Optimization Algorithms in Physics*, which can serve as an appendix for the newcomer to this field of computational physics or for undergraduate students. The reason why we found it necessary to compose another book in this field with a greater focus is the fact that the application of optimization methods is one of the strongest growing fields in physics. The main reasons for these current developments are the following key factors:

First of all great progress has been made in the development of new combinatorial optimization methods in computer science. Using these sophisticated approaches, much larger system sizes of the corresponding physical systems can be treated. For many models the systems sizes which were accessible before, were too small to obtain reliable and significant data. However, this is now possible. In this way computer science has helped physics.

But knowledge transfer also works the other way round. Physics provides still new insights and methods of treating optimization problems, such as the earlier invention of the simulated annealing technique. Recent algorithmic developments in physics are, e.g., the extremal optimization method or the hysteric optimization approach, both covered in this book.

Moreover, phase transitions were recently found in “classical” optimization problems within theoretical computer science, during the study of suitably parameterized ensembles. These phase transitions very often coincide with peaks of the running time or with changes of the typical-case complexity from polynomial to exponential. As well as the gain from taking the physical viewpoint, by mapping the optimization problems to physical systems and applying methods from statistical physics, it is possible to obtain many results, which have not been found with traditional mathematical techniques. This is true also for the analysis of the typical-case complexity of (random) algorithms.

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Finally: All benefit from the increasing power of computers. Despite all predictions, the speed of the hardware still seems to grow exponentially fast, making the application of optimizations methods more and more valuable.

Thus the aim of this book is to promote progress in the fields given above. Physicists will become familiar with the huge progress still taking place in the development of algorithmic techniques. On the other hand, the new developments of physically inspired algorithms can be very useful in computer science as well. In particular the application of physical methods in the field of phase transitions seems to be a very promising field for the next decade.

Currently, the interactions between different communities, namely mathematics, computer science, biology, economy and physics are still too weak. Only by gathering researchers from these different groups and trying to find a common language, can real progress be achieved. All problems, algorithms and results are presented here in a pedagogical way, which makes the information available to a broad audience. This is the main purpose of this collection of papers.

The book contains three main parts. In the first part, we focus on applications of optimization algorithms to problems from physics. The standard way of solving computational problems in statistical physics is to use a Monte Carlo simulation. In his contribution, Werner Krauth shows that by using modern cluster algorithms, many previously inaccessible models can be treated at low temperatures (obtaining low, i.e., minimum energies) or respectively, high densities. He studies as examples the phase separation in binary mixtures and the application of the algorithm to monomer-dimer models. Next, Olivier Martin surveys algorithms for Ising spin-glass ground-state calculations and he explains one new Monte Carlo algorithm in detail. It is a cluster method based on the real-space renormalization group.

Monte Carlo methods, like those shown in the first two contributions, are very efficient and have a wide range of applicability, but they do not guarantee to find a global optimum solution. In contrast, the Branch-and-Cut approach is an exact algorithm. It is presented by Frauke Liers, Michael Jünger, Gerhard Reinelt and Giovanni Rinaldi. They explain the method for an application to the max-cut problem, which is used here for the ground-state calculation of three-dimensional Ising spin glasses.

Another important class of problems in statistical physics is the random-field Ising model. Alan Middleton explains how one can calculate ground states using push/relabel algorithms in polynomial time, how these algorithms perform near phase transitions and how one can use it to characterize the ground-state landscape of the random-field model. In the last chapter of the first part, Jean-Christian Anglès d'Auriac describes a new method for calculating the partition function and other thermodynamic quantities of the infinite-state Potts model with random bonds using a combinatorial optimization algorithm. The latter is based on the concept of submodular functions, which might also prove useful in a number of other applications in the near future.

The second part is dedicated to the study of phase transitions in combinatorial optimization problems. First, Martin Weigt introduces the Satisfiability Problem (SAT), the most fundamental problem in computational complexity theory. He then shows how one can generate large SAT formulas which have a solution but where the solution is hard to find for local algorithms like Walksat. This behavior can be understood by solving the corresponding physical problem analytically by using techniques from statistical mechanics. Simona Cocco, Liat Ein-Dor and Remi Monasson show how one can calculate the typical running time of exact backtracking algorithms for SAT and for the coloring problem. The basic idea is to investigate the dynamics of the algorithm moving in the phase diagram of the problem. Finally, Riccardo Zecchina presents the currently fastest Algorithm for SAT, the Survey Propagation algorithm, which allows to solve SAT instances near the SAT-UNSAT phase transition of systems having 10^6 variables. The method is based on the cavity approach, an analytical technique used to study mean-field-like disordered systems in statistical physics. Nevertheless, his presentation is solely based on probability theory, making it also very accessible to non-physicists.

The third part of this book is on new heuristics and interdisciplinary applications. Károly Pál presents an optimization method which is inspired by a physical technique, the measurement of hysteresis in a magnetic system. The basic idea is to demagnetize a system by performing hysteresis loops with continuously decreasing magnitude. He presents the algorithm in a very general style, which in principle allows arbitrary applications. As examples, results for spin glasses and the traveling salesman problem are shown. Stefan Boettcher explains another very general algorithm, the extremal optimization algorithm. Its basic idea is very simple and similar to genetic algorithms. The latter ones usually have many free parameters, which must be tuned to obtain an efficient algorithm. Extremal optimization has the advantage that it is, in the simplest variant, absolutely parameter free. Another major difference in comparison with genetic algorithms is that fitness values are not assigned to different configurations but to different particles of one configuration. Application to graph coloring, spin glasses and image matching are given.

The last two contributions contain applications from Molecular Biology. After providing some biological background, Alexander Hartmann explains alignment algorithms, which are used to compare biological sequences by applying a shortest-path algorithm. As an application, a method to obtain the rare-event tail of the statistics of protein alignments is presented. Finally, Ulrich Hansmann reviews methods used to solve protein-folding problems via energy minimization and in particular explains energy-landscape paving. The basic idea is that one initially modifies the energy landscape such that the global minimum is easier to find. During the simulation, the energy landscape gradually approaches the ordinal one. Furthermore, the algorithm tries to avoid previously visited regions, if the energy is not low enough. Various results for the influence of the temperature on helix formation are also shown.

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